Myle Akshay Kiran, Chemistry and Biomedicine 2018, Volume 8
DOI: 10.4066/2249-622X-C4-012

Investigations and computation of chemicals used in advanced technological research for the prevention of diseases in present scenario

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Investigations of Chemicals - computational investigations of hydrogen bonding, with regard to the most common red shift in the vibrational frequency, as well as the less common blue shift in several hydrogen bonded systems. thereby generating new insight into both types of the frequency shifts. Thus, the frequency shifts in X—H—Y hydrogen bonded systems at different H—Y distances are shown to correlate well with the Mulliken charges on H and Y, with the positive and negative charges on Y correlating with the blue and red shift of the frequency of X—H vibration, respectively. The role played by charge transfers at other parts of the interacting system is also discussed.

Advanced computation - advances in computing have facilitated major progress in computational chemistry and biochemistry, computational materials design, computational fluid dynamics, process synthesis, planning and scheduling, model-based process control, fault diagnosis, and real-time process optimization. Investigations by involving indicators - investigations have revealed something of more significance By examining lower-consequence, higher-frequency occurrences, companies may avoid those rare incidents that cause major consequences. The two most significant roles incident investigations can play in comprehensive process.

Computation of electrons - electronic structure is the state of motion of electrons in an electrostatic field created by stationary nuclei. The term encompass both the wave functions of the electrons and the energies associated with them. Electronic structure is obtained by solving quantum mechanical equations for the aforementioned clamped-nuclei problem. Electronic structure problems arise from the Born–Oppenheimer approximation. Along with nuclear dynamics problem, electronic structure problem is one of the two steps to study quantum mechanical motion of a molecular system, we design the molecule with protein structure, lead optimization is multi optimization, the rate at which drug action undergoes in solubility and Computational methods and techniques differently we can predict it, it can help by the structure based drug discovery and Computational analysis, Designing chemicals - Designing approaches for particular fragments site for screening and available solids, Pharmacophores, fragment-based properties, profile similarity and structural similarity, and theoretical conditions when working with protein structures, ligands conformation energies are the important as protein ligands interactions energies, ligands based modeling methods, are very active and effinity when having protein structures.

Speaker Biography

Myle Akshay Kiran is an International Research Scholar and Doctor of Pharmacy at the Jawaharlal Nehru Technological University at India. His area of research is in immunization vaccine. He has been the Editor of many Journal publications and presented his research work at various conferences.

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